Conventions, Accuracy Metrics, Classification, Regression

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IIT Gandhinagar

Demo

- Complete PoseNet Demo

Demo

- Complete PoseNet Demo
- Blog post from Google

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- Rock Paper Scissors

Revision: What is Machine Learning

"Field of study that gives computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

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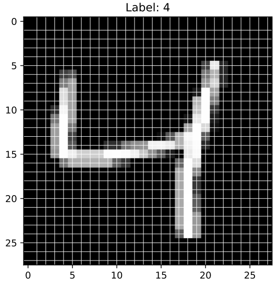
Let us work on the digit recognition problem.

Notebook: rule-based-vs-ml.html



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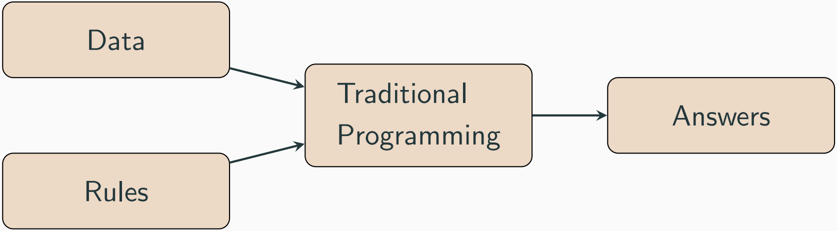
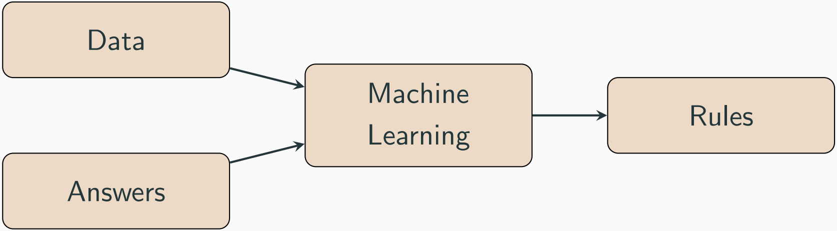
- There can be some cases of 4 where the width of each stroke is different

Traditional Programming vs Machine Learning

Traditional Programming



Machine Learning



Revision: What is Machine Learning

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E." - Tom Mitchell

First ML Task: Grocery store tomato quality prediction

Problem statement: You want to predict the quality of a tomato given its visual features.

Dataset

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

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Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour

Dataset

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Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour
- Texture

Sample Dataset

Here is our example dataset with tomato features:

Sample	**Colour**	**Size**	**Texture**	**Condition**
1	Orange	Small	Smooth	Good
2	Red	Small	Rough	Good
3	Orange	Medium	Smooth	Bad
4	Yellow	Large	Smooth	Bad

Useful Features

Is the sample number a useful feature for predicting quality of a tomato?

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Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it.

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Let us modify our data table for now.

Colour	**Size**	**Texture**	**Condition**
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

Training Set

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
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The training set consists of two parts:

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The training set consists of two parts:

1. Features (Input Variables)
2. Output or Response Variable

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1. Feature matrix ($\mathbf{X} \in \mathbb{R}^{n \times d}$) containing data of n samples each of which is d dimensional.

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We call this matrix as $\mathcal{D}$, containing:

1. Feature matrix ($\mathbf{X} \in \mathbb{R}^{n \times d}$) containing data of n samples each of which is d dimensional.
2. Output vector ($\mathbf{y} \in \mathbb{R}^{n}$) containing output variable for n samples.

Data Matrix Details

- Feature matrix: $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix}$ where $\mathbf{x}_i \in \mathbb{R}^d$

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- Example (after encoding): $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ (Orange=1, Small=0, Smooth=1)

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- Example (after encoding): $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ (Orange=1, Small=0, Smooth=1)
- Complete dataset: $\mathcal{D} = \{(\mathbf{x}_i^\top, y_i)\}_{i=1}^n$

Prediction Task

Estimate condition for unseen tomatoes (#5, 6) based on data set.

Colour	**Size**	**Texture**	**Condition**
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

Testing Set

Testing set is similar to training set, but, does not contain labels for output variable.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
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Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

Prediction Task

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Prediction Task

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2. From Training Dataset
3. To Predict the condition for the Testing set

Colour	Size	Texture	Condition
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Red	Small	Rough	Good
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Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

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- A: Ideally, no!
- Ideally - we want to predict "well" on all possible inputs. But, can we test that?
- No! Since, the test set is only a sample from all possible inputs.

Generalisation

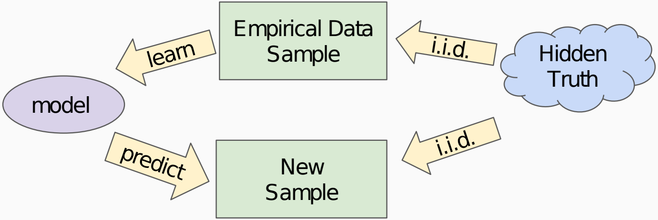

Image courtesy Google ML crash course

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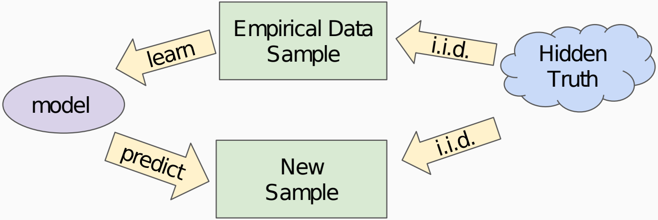

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Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

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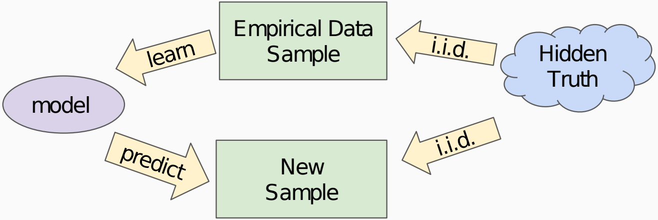

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More discussion later once we study bias and variance

Second ML Task: Predict energy consumption of campus

Question: What factors does the campus energy consumption depend on?

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# People	**Temp (C)**	**Energy (kWh)**
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

Classification vs Regression

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  - Examples - Predicting:
    - How much energy will campus consume?
    - How much rainfall will fall?

Metrics for Classification

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} \qquad \text{Ground Truth } (\mathbf{y}) \quad \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Bad} \end{pmatrix}$$

Ground Truth: From the actual training set
Prediction: Made by the model

Accuracy

$$
\begin{array}{cc}
 & \text{Prediction } (\hat{y}) \\
\begin{array}{c} \checkmark \\ \checkmark \\ \\ \\ \checkmark \end{array} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}
\end{array}
\qquad
\begin{array}{c}
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$$

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$$\begin{aligned} \text{Accuracy} &= \frac{|\{i : y_i = \hat{y}_i\}|}{n} \\ &= \frac{3}{5} = 0.6 \end{aligned}$$

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- **Alternative: Indicator function notation**

$$\text{Accuracy} = \frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

$$\text{where } \mathbf{1}[\text{condition}] = \begin{cases} 1 & \text{if condition is true} \\ 0 & \text{if condition is false} \end{cases}$$

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- Both notations are mathematically equivalent and commonly used in ML literature

Types of Data: Imbalanced Classes

$$\begin{array}{r} \text{1 sample} \left\{ \vphantom{\text{Bad}} \right. \\ \text{100 samples} \left\{ \begin{array}{c} \\ \\ \\ \\ \end{array} \right. \end{array} \begin{pmatrix} \text{Bad} \\ \text{Good} \\ \text{Good} \\ \dots \\ \text{Good} \end{pmatrix}$$

Imbalanced Classes

Types of Data: Imbalanced Classes

$$\begin{array}{r} \text{1 sample}\left\{ \vphantom{\text{Bad}} \right. \\ \text{100 samples}\left\{ \vphantom{\begin{array}{c}\text{Good}\\\text{Good}\\\dots\\\text{Good}\end{array}} \right. \end{array} \begin{pmatrix} \text{Bad} \\ \text{Good} \\ \text{Good} \\ \dots \\ \text{Good} \end{pmatrix} \qquad \text{Imbalanced Classes}$$

Cases for this:

- Cancer Screening

Types of Data: Imbalanced Classes

$$\begin{array}{r} 1\text{ sample}\ \{ \\ 100\text{ samples}\ \left\{\begin{array}{c} \\ \\ \\ \\ \end{array}\right. \end{array} \begin{pmatrix} \text{Bad} \\ \text{Good} \\ \text{Good} \\ \dots \\ \text{Good} \end{pmatrix} \qquad \text{Imbalanced Classes}$$

Cases for this:

- Cancer Screening
- Planet Detection

Accuracy Metrics: Precision

$$
\begin{array}{cc}
\begin{array}{l} \rightarrow \checkmark \\ \rightarrow \checkmark \\ \rightarrow \\ \rightarrow \\ \end{array}
\overset{\text{Prediction } (\hat{y})}{\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}}
&
\overset{\text{Ground Truth } (\mathbf{y})}{\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}}
\end{array}
$$

$$
\text{Precision} = \frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : \hat{y}_i = \text{Good}\}|} = \frac{2}{4} = 0.5
$$

"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

Accuracy Metrics: Precision

$$
\begin{array}{ll}
 & \text{Prediction } (\hat{y}) \\
\begin{array}{l} \rightarrow \checkmark \\ \rightarrow \checkmark \\ \rightarrow \\ \rightarrow \\ \end{array} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}
\end{array}
\qquad\qquad
\begin{array}{c}
\text{Ground Truth } (\mathbf{y}) \\
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}
\end{array}
$$

$$
\text{Precision} = \frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : \hat{y}_i = \text{Good}\}|} = \frac{2}{4} = 0.5
$$

"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

Accuracy Metrics: Recall

$$\begin{array}{cc} & \text{Prediction } (\hat{y}) \\ \rightarrow \checkmark & \\ \rightarrow \checkmark & \\ & \\ & \\ \rightarrow & \end{array} \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} \qquad \begin{array}{c} \text{Ground Truth } (\mathbf{y}) \end{array} \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}$$

$$\text{Recall} = \frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : y_i = \text{Good}\}|} = \frac{2}{3} = 0.67$$

"the fraction of the total amount of relevant instances that were actually retrieved"

Types of Data: Imbalanced Classes

Given predictions of whether a tissue is cancerous or not ($n = 100$).

$$\begin{array}{c} \\ \rightarrow \\ \\ \\ \\ \\ \end{array}\begin{array}{c} \text{Prediction } (\hat{y}) \\ \begin{pmatrix} \text{Yes} \\ \text{No} \\ \text{No} \\ \dots \\ \text{No} \end{pmatrix} \end{array} \qquad \begin{array}{c} \\ \\ \\ \\ \\ \rightarrow \end{array}\begin{array}{c} \text{Ground Truth } (\mathbf{y}) \\ \begin{pmatrix} \text{No} \\ \text{No} \\ \dots \\ \text{No} \\ \text{Yes} \end{pmatrix} \end{array}$$

Types of Data: Imbalanced Classes

Given predictions of whether a tissue is cancerous or not ($n = 100$).

$$\begin{array}{cc} & \text{Prediction } (\hat{y}) \\ \rightarrow & \left(\begin{array}{c} \text{Yes} \\ \text{No} \\ \text{No} \\ \ldots \\ \text{No} \end{array}\right) \end{array} \qquad \begin{array}{cc} & \text{Ground Truth } (\mathbf{y}) \\ & \left(\begin{array}{c} \text{No} \\ \text{No} \\ \ldots \\ \text{No} \\ \text{Yes} \end{array}\right) \\ \end{array}$$

$$\text{Accuracy} = \frac{98}{100} = 0.98$$

$$\text{Recall} = \frac{0}{1} = 0$$

$$\text{Precision} = \frac{0}{1} = 0$$

Accuracy Metrics: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	0	1
	No	1	98

Accuracy Metrics: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	0	1
	No	1	98

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

Accuracy Metric: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

$$\text{Precision} = \frac{\text{TP}}{\text{TP+FP}}$$

Accuracy Metric: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

$$\text{Precision} = \frac{\text{TP}}{\text{TP}+\text{FP}}$$

Accuracy Metric: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

$$\text{Recall} = \frac{\text{TP}}{\text{TP}+\text{FN}}$$

Accuracy Metric: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

$$\text{Recall} = \frac{\text{TP}}{\text{TP}+\text{FN}}$$

Accuracy Metrics: F-Score

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

$$\mathrm{F}- \text{ Score} = \frac{2\times \text{ Precision } \times \text{ Recall}}{\text{Precision } + \text{ Recall}}$$

Accuracy Metrics: Matthew's Correlation Coefficient

		Ground Truth	
		Yes	No
Predicted	Yes	True Positive	False Positive
	No	False Negative	True Negative

Matthew's correlation coefficient $= \frac{\text{TP}\times\text{TN}-\text{FP}\times\text{FN}}{\sqrt{(\text{TP}+\text{FP})(\text{TP}+\text{FN})(\text{TN}+\text{FP})(\text{TN}+\text{FN})}}$

Accuracy Metrics: Example

For the data given below, calculate:

$$\begin{array}{r c} & \begin{array}{cc} \text{G.T. Positive} & \text{G.T. Negative} \end{array} \\ \begin{array}{r} \text{Pred Positive} \\ \text{Pred Negative} \end{array} & \begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix} \end{array}$$

Precision $=$?

Recall $=$?

F-Score $=$?

Matthew's Coeff. $=$?

Accuracy Metrics: Answer

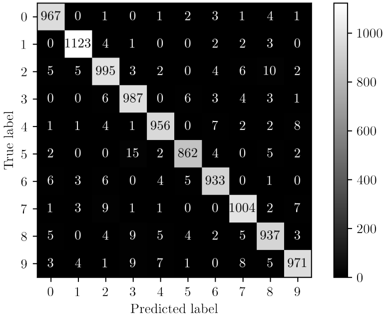
For the same data

$$\begin{array}{r c} & \begin{array}{cc} \text{G.T. Positive} & \text{G.T. Negative} \end{array} \\ \begin{array}{r} \text{Pred Positive} \\ \text{Pred Positive} \end{array} & \begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix} \end{array}$$

Precision $= \frac{90}{94}$
Recall $= \frac{90}{91}$
F-Score $= 0.9524$
Matthew's Coeff. $= 0.14$

Confusion Matrix for multi-class classification

Notebook: confusion-mnist.html



Metrics for Regression MSE & MAE

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad \text{Ground Truth } (\mathbf{y}) \quad \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$$

$$\text{Mean Squared Error (MSE)} = \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n}$$

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\text{MSE}}$$

Accuracy Metrics: MAE & ME

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad \text{Ground Truth} \quad \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$$

$$\text{Mean Absolute Error (MAE)} = \frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n}$$

$$\text{Mean Error} = \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Accuracy Metrics: MAE & ME

Prediction ($\hat{y}$)	Ground Truth
$\begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$

$$\text{Mean Absolute Error (MAE)} = \frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n}$$

$$\text{Mean Error} = \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Is there any downside with using mean error?

Accuracy Metrics: MAE & ME

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad \text{Ground Truth} \quad \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$$

$$\text{Mean Absolute Error (MAE)} = \frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n}$$

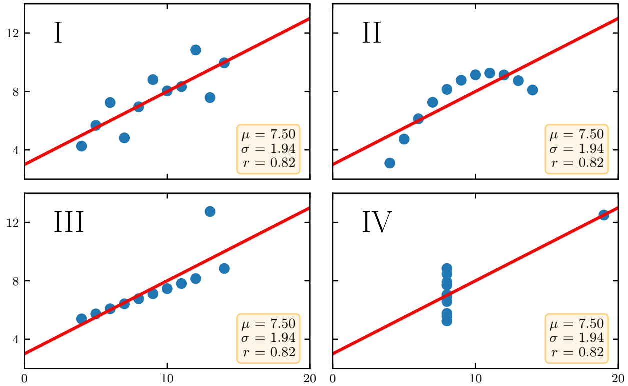
$$\text{Mean Error} = \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Is there any downside with using mean error?

Errors can get cancelled out

The Importance of Plotting

Notebook: anscombe.html



Anscombe's Quartet

Dummy Baselines

Notebook: dummy-baselines.html

The Importance of Plotting

Property	Value	Across datasets
mean(X)	9	exact
mean(Y)	7.5	up to 3 decimal places
Linear regression line	$y = 3.00 + 0.500x$	up to 2 decimal places